CLAIMS

1. A parallel computing method for executing calculation of the Hartree-Fock method in a molecular orbital method, comprising the steps of:

using a computer cluster made up of a plurality of computers;

dividing a density matrix into multiple density submatrixes and distributing the multiple density submatrixes to the multiple computers and storing therein; and

executing calculation processes on the density submatrixes in each of the computers while sequentially transferring the multiple density submatrixes between the multiple computers.

2. The method according to Claim 1, wherein a duplication of the density matrix is used, and the density matrix and the duplication are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers to thereby reduce calculation of integrals.

3. The method according to Claim 1, wherein the density matrix and duplications of the density matrix, four in total, are used, and the density matrix and the duplications are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \Leftrightarrow (tu|rs)$ in two-electron integration.

4. The method according to Claim 1, further comprising the step of:

partially executing two-electron integration in each of the computers and updating the stored density submatrixes based on the result of the two-electron integration.

5. The method according to Claim 4, wherein a duplication of the density matrix is used, and the density matrix and the duplication are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers to thereby reduce calculation of integrals.

6. The method according to Claim 4, wherein the density matrix and duplications of the density matrix, four in total, are used, and the density matrix and the duplications are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \Leftrightarrow (tu|rs)$ in two-electron integration.

7. A parallel computing system for executing calculation of the Hartree-Fock method in a molecular orbital method, comprising:

a computer cluster made up of a plurality of computers,

each of the computers comprising a matrix storage for storing density submatrixes which are divided from a density matrix; a transfer controller for performing transmission and reception of the density submatrixes with respect to the other computers in the computer cluster; and a calculation processor for performing a calculation on the density submatrix stored in the matrix storage,

wherein calculation processes on the density submatrixes are executed in each of the computers while the multiple density submatrixes are being sequentially transferred between the multiple computers.

8. The system according to Claim 7, the density matrix and a duplication of the density matrix are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers to thereby reduce

calculation of integrals.

9. The system according to Claim 7, wherein the density matrix and duplications of the density matrix, four in total, are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \Leftrightarrow (tu|rs)$ in two-electron integration.

10. The system according to Claim 7, wherein the calculation processor partially executes two-electron integration and the density submatrix in the matrix storage is updated based on the result of two-electron integration.

11. The system according to Claim 10, wherein the density matrix and a duplication of the density matrix are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers to thereby reduce calculation of integrals.

12. The system according to Claim 10, wherein the density matrix and duplications of the density matrix, four in total, are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \Leftrightarrow (tu|rs)$ in two-electron integration.

13. A program causing a computer at each node in a computer cluster constituted by a plurality of nodes, to function as:

a matrix storage for storing density submatrixes which are divided from a density matrix; a transfer controller for performing transmission and reception of

the density submatrixes with respect to the other nodes in the computer cluster; and a calculation processor for performing a calculation on the density submatrix stored in the matrix storage,

whereby calculation processes on the density submatrixes are executed at each of the nodes while the multiple density submatrixes are being sequentially transferred between the multiple nodes.

14. A recording medium which is readable by computers and has the program defined in Claim 13 stored therein.